

Isoflupredone, bis-MO-tris-TMS

Inchi: InChI=1S/C32H57FN2O5Si3/c1-29-18-16-24(34-36-3)20-23(29)14-15-26-25-17-19-31(40-41-32)33-35-37-38-39-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: YIWPTVOOWPWARJ-XZVCHNANSA-N
Formula: C32H57FN2O5Si3
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C3CCC(O[Si](C)(C)C)(C(CO[Si](C)(C)C)=NOC)C3(C)C
Mol. weight [g/mol]: 653.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Crippen Method
logp	8.094		Crippen Method
rinpol	3000.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558055&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/42-175-1/Isoflupredone-bis-MO-tris-TMS.pdf>

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